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Progress Report to JSEP

The remarkably well-ordered morphology of faceted Si(113) surfaces was discovered under JSEP sponsorship in 1994 and has since been the subject of extensive research. In past years, our quantitative characterization of the equilibrium thermal behavior has validated the description of thermal faceting of stepped surfaces as a phase-separation of orientational phases. The construction of orientational phase diagram was performed with unprecedented precision, which enabled fine distinctions to be made between the phase separation of stepped Si(113) surfaces and that of other semiconductor and metal surfaces. Namely, the phase separation of stepped Si(113) surfaces is effected by the competition of a long-ranged repulsion between steps and a short-ranged attraction, a novel mechanism of current theoretical interest. In the 1996-1997 academic year, we have concluded the extension of our studies of the orientational phase diagram into previously unexplored azimuthal orientations vicinal to (113). Faceting transitions are observed on all surface orientations studied, which commonly are accompanied by anomalous step fluctuations and share similar characteristics of the orientational phase boundary. However, due to the strong anisotropy inherent to crystal surfaces, the transition temperatures for different azimuths are very different. We expect these refined observations to be accommodated in recently-proposed theories of thermal faceting.

Another area of current research on thermal faceting concerns its kinetics. The time-dependent formation of well-ordered array of facets has been a long-standing problem of metallurgy, and more recently there has been a renewed interest in the subject facilitated mainly by the development of high-resolution experimental tools. Most investigations prior to ours have either revealed discrepancies from classical theories of faceting kinetics or remained inconclusive as to the applicability of such thoeries. Our own investigation, on the other hand, has proved more rewarding in that the length and time scales of ordering on stepped Si(113) surfaces nicely match our experimental capabilities, which utilize the methods of time-resolved x-ray scattering. Especially, the use of a CCD area detector in a grazing-incidence reflection geometry enabled us to follow the evolution of faceting in real time, in situ, and in two (highly anisotropic) spatial dimensions. The length of ordered facets typically on the order of 1-30μm, as well as the separation between facets on the order of 30-150nm, was measured as a function of time during an evolution towards ordered faceted morphology. They evolve as power laws versus time, with the length of facets varying as the third power of their width throughout the coarsening regime. These results signify the novel observation of anisotropic dynamic scaling, and endorse a very recent theory of faceting kinetics that focuses on the thermal fluctuation of step bunches between facets and takes the collision between adjacent step bunches as the rate-limiting mechanism of facet growth.

The coarsening regime is followed in time by the ordering regime in which a well-defined facet width is achieved across the entire surface. The periodic array of grooves (composed of facets and step bunches) extends to tens of μm in length. Our characterization of the temperature dependence of the equilibrium periodicity presents evidence that reduction of elastic energy is responsible for the formation of well-defined groove periodicity on the submicron length scale. Interesting possibilities exist that utilize these grooved surfaces as templates for nanoscale wire formation.

We have also applied our experience with the techniques of time-resolved x-ray scattering

to the initial stage of lattice-mismatched, hetero-epitaxial growth of Ge on Si(001). Our investigation was motivated by the recent discovery of a self-organized array of dislocation-free islands on this and related systems, which has since been followed by intensive experimental and theoretical studies. Underlying the intense attention paid to this phenomenon is the expectation that the array of quantum dots self-organized on strained semiconductors may ultimately be utilized in opto-electronic devices. The submicron size of these dots presents self-organization as a promising route to nanofabrication. The worldwide effort to improve the uniformity of the grown dots is still underway, as it is to understand the physical mechanisms of self-organization from a scientific standpoint. Our characterization of the initial growth process has contributed detailed, systematic, and quantitative data to this effort, which previously have not been available. Specifically, we have measured the size and the areal density of the dislocation-free islands versus time, during MBE deposition at various temperatures and deposition rates. We also have distinguished the nucleation characteristics of dislocated islands (that do not self-organize) from that of the dislocation-free islands. A formalism to numerically solve rate equations of this complex kinetic process currently exists, and a collaboration with a theoretical research group is in progress to extract from our data the relevant energetics for the Ge/Si(001) system.

The following publications have been sponsored by JSEP in the 1996-1997 academic year.

[1] S. G. J. Mochrie, S. Song, M. Yoon, D. L. Abernathy, and G. B. Stephenson, "Faceting of stepped Si(113) surfaces: Self-assembly of nanoscale gratings" Physica B **221**, 105 (1996).

[2] S. Song, M. Yoon, S. G. J. Mochrie, G. B. Stephenson, and S. T. Milner, "Faceting kinetics of stepped Si(113) surfaces: Dynamic scaling and nano-scale grooves" Surf. Sci. **372**, 37 (1997).

[3] M. J. Fasolka, D. J. Harris, A. M. Mayes, M. Yoon, and S. G. J. Mochrie, "Observed substrate topography-mediated lateral patterning of diblock copolymer films" Phys. Rev. Lett. **79**, 3018 (1997).

[4] M. Yoon, S. G. J. Mochrie, M. W. Tate, S. M. Gruner, and E. F. Eikenberry, "Anisotropic coarsening of periodic grooves: Time-resolved x-ray scattering" Phys. Rev. Lett. **79**, in print (1997).

[5] M. Yoon, "X-ray scattering studies of self-organized nanoscale-structures on semiconductor surfaces" Ph.D thesis, MIT (1997).

[6] M. Yoon, S. G. J. Mochrie, M. W. Tate, S. M. Gruner, and E. F. Eikenberry, "Periodic faceting of a Si(113) surface miscut towards $[1\bar{1}0]$" (to be published).

[7] M. Yoon and S. G. J. Mochrie, "High-temperature disordering of the Si(001) (2x1) reconstruction" (to be published).

[8] M. Yoon and S. G. J. Mochrie, "Growth of Ge Islands on Si(001): In-situ x-ray scattering" (to be published).

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